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Quasistatic Cracks and Minimal Energy Surfaces

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We compare the roughness of minimal energy (ME) surfaces and scalar "quasistatic" fracture (SQF) surfaces. Two-dimensional ME and SQF surfaces have *the same roughness scaling*, $w \sim L^{\zeta}$ (L is the system size) with $\zeta = \frac{2}{3}$. The 3*d* ME and SQF results at strong disorder are consistent with the random-bond Ising exponent $\zeta(d \geq 3) \approx 0.21(5 - d)$ (d is the bulk dimension). However, 3*d* SQF surfaces are *rougher* than ME surfaces due to a larger prefactor. ME surfaces undergo a "weakly rough" to "algebraically rough" transition in 3*d*, suggesting a similar behavior in fracture. [S0031-9007(97)04993-4]

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Fracture [1] continues to attract the attention of the materials theory community, with the full spectrum of theoretical tools currently being applied to its analysis [1–9]. Cracks are usually self-affine and their roughness can be characterized by a roughness exponent (ζ), which may take on a few distinct values [7–9] (here, we calculate the "out-of-plane roughness" of fracture surfaces). However, a debate continues about whether or not fracture surfaces are ever generated by "quasistatic" processes [2,7,8,10]. A quasistatic fracture process is one in which the stress field is always close to equilibrium. For this to be true, damage must evolve much more slowly than the time required for the stress field to equilibrate. Slow crack growth and high cycle fatigue are expected to be in this limit. As well as their fundamental interest, the latter processes are of enormous industrial importance. Bouchaud *et al.* [8] argue that at short length scales (as probed by, e.g., scanning tunneling microscopy) quasistatic processes dominate, while at longer length scales dynamical processes are of primary importance. Here, we present extensive numerical results on the topology of quasistatic fracture surfaces in random fuse networks. We also compare these fracture surfaces with minimal energy surfaces in the *same networks*. Using fast optimization methods, we are able to simulate the latter interfaces for large system sizes.

Surprisingly [11], the roughness exponent of minimal energy (ME) surfaces and scalar quasistatic brittle fracture (SQF) surfaces have been shown to be close in two dimensions. This is surprising because a minimal energy surface is the surface of minimum energy in, for example, an Ising model with random bonds (see below), which seems to have little to do with fracture. Nevertheless, there is some experimental evidence that this holds in two dimensions [12]. We present precise numerical confirmation of the equivalence of ME and SQF roughness exponents in two dimensions. We analyze networks with either continuous or discrete disorder and find the same size dependence in all cases, in contrast to previous suggestions that discrete disorder is special [13].

In three dimensions, our calculations are for ME and SQF surfaces of the cubic lattice in the {100} direction. We choose the low energy, {100} direction as it is more typical of the orientation of fracture surfaces. It has been recently claimed that vector quasistatic fracture (VQF) surfaces are logarithmically rough at *weak disorder* [10]. In the same paper, it was stated that SQF are algebraically rough in the same disorder regime. Since this result is at odds with the experimental data [8], which are naturally for the vector case, it was further suggested that quasistatic fracture is not relevant in real experiments. The latter statement is difficult to believe, for example, in the case of high cycle fatigue, in which the time to failure is days to years. One possible reason for this dichotomy is that the calculations of Ref. [10] may apply at weak disorder and that there may be a transition to an algebraically rough phase as disorder increases. To illustrate that this may occur even in the scalar case, we present extensive data confirming our claim [14] that *at weak disorder* ME surfaces in the {100} orientation are quite flat (probably logarithmically rough), while at strong disorder they become algebraically rough.

The simplest realization of a ME surface is a domain wall in a random-bond Ising model with Hamiltonian $H = -\sum J_{ij} S_i S_j$, where $S_i = \pm 1$ and J_{ij} are random but non-negative. A domain wall is imposed by fixing one face of a square or cubic lattice to be positive and the opposite face to be negative. It was only recently realized that the problem of finding the minimal energy surface (domain wall) is equivalent to an important and well-known problem in graph theory (the min-cut/max-flow problem) [14,15]. In the flow problem, each bond of the lattice has a "flow capacity" ($c_{ij} = 2J_{ij}$) and, once the flow capacity of a bond has been reached, the excess flow must be shunted along alternative paths (bonds). The

domain wall energy is equal to the maximum flow that can be pushed through the network without exceeding any of the capacities. Fast, exact algorithms are available for the flow problem and we have developed and applied these algorithms previously [14]. Here, we extend these calculations, and compare them with results for SQF surfaces.

The fuse network is an electrical network (e.g., a simple cubic lattice) in which each bond is a resistor which fails when more than a threshold current i_{ij} amp passes through it. We use the standard *hottest bond* algorithm for calculating fracture surfaces in the fuse network. These electrical networks usually capture many of the essential features of failure problems and have become a paradigm in the area [2].

To quantitatively compare fracture and minimal energy surfaces, we set the critical current for the failure of a fuse (i_{ij}) to the flow capacity used in the minimal surface calculation (i.e., $c_{ij} = i_{ij}$). The simple physical difference between the two cases is that in the fuse network a bond carries no current once i_{ij} is exceeded (it breaks), while in the minimal surface case, a bond continues to carry its threshold capacity $i_{ij} = c_{ij}$ even after its threshold is exceeded (it "yields" but does not break). The latter case corresponds to a "perfectly plastic" response. In all cases, we have done calculations for two types of disorder: random dilution, with probability p of a bond being present with $2J_{ij} = c_{ij} = i_{ij} = 1$; and, for a uniform distribution, with $2J_{ij} = c_{ij} = i_{ij}$ drawn from a uniform distribution with mean 1 and extending from $1 - R$ to $1 + R$.

Results for two dimensions are presented in Figs. 1 and 2. In Figs. 1(a) dilution disorder) and 2(a) (continuous disorder), we present data for the size dependence of the interface roughness or "width" $w \sim c(p)L^{\zeta}$, $w^2 = \langle h(x) - \langle h(x)\rangle\rangle^2$ [$h(x)$ describes the interface position for a given disorder configuration]. The data in these figures demonstrate that the roughness exponent of minimal energy surfaces and scalar fracture surfaces are asymptotically the same in two dimensions. Thus, as suggested previously [11], the roughness exponent takes the value $\zeta = \frac{2}{3}$ [dotted line in Figs. 1(a) and 2(a)], which is exact for ME's [16]. In Fig. 1(b), we show that ME and SQF surfaces are rough for arbitrarily weak dilution disorder in two dimensions. We also calculated the roughness of cracks grown from an initial notch and find results consistent with Figs. 1(a) and 2(a). For a given realization, ME's and SQF surfaces may still be quite different and have different roughness [see Fig. 2(b)]. We found that for dilution disorder ME and SQF paths are more similar, but for a continuous distribution they are usually different, with the SQF surfaces being rougher. [This can be seen in Fig. 2(b).] This is due to the distributed "damage" generated by the SQF process, with this process being more important for continuous disorder than for the dilution case.

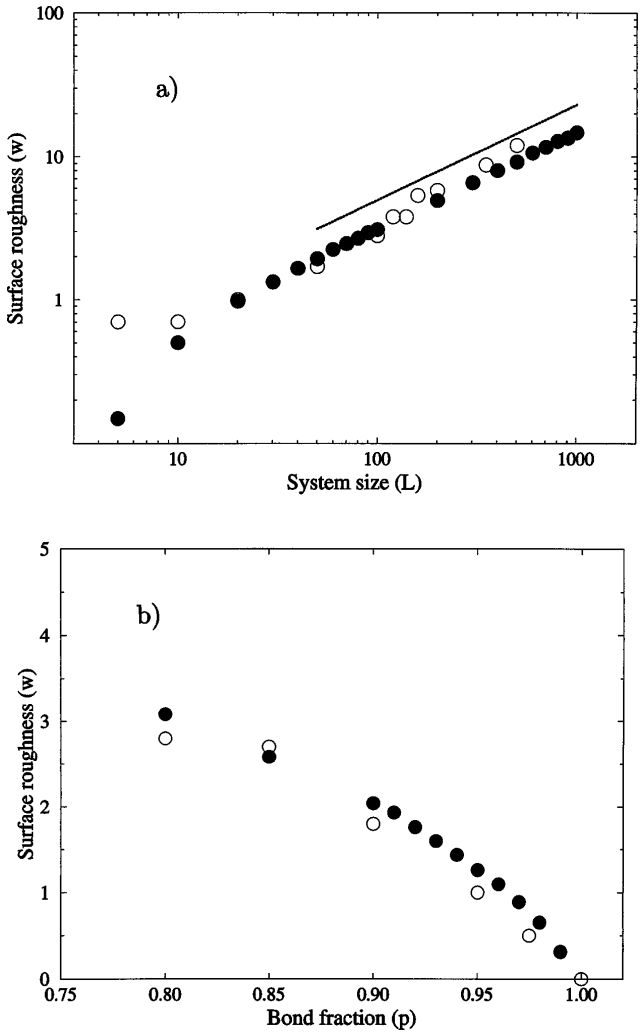

FIG. 1. The roughness w of scalar quasistatic fracture (SQF) surfaces and minimal energy (ME) surfaces in the {10} orientation of square lattices with *dilution* (discrete) disorder. (a) Log-log plot of w as a function of system size L at $p = 0.80$: SQF (open circles); ME (filled circles). The dotted line has slope $\zeta = \frac{2}{3}$. Boundary conditions were periodic in the perpendicular direction. For SQF, the number of configurations in the averages, N, varied from $N = 10$ for $L = 500$ to $N = 256$ for $L = 10$, while for the ME, we used $N = 100$ for $L = 1000$ up to $N = 5000$ for $L = 50$. (b) The dependence of w on disorder for SQF ($L = 100$, $N = 30$—open circles) and ME ($L = 100$, $N = 5000$—filled circles).

Results of simulations in three dimensions are presented in Fig. 3. Figure 3(a) presents data for the roughness of SQF and ME surfaces in 40^3 {100} cubic lattices with dilution disorder. We use periodic boundary conditions in one direction, and free ones in the other. Two differences between these data and the behavior in two dimensions [Fig. 1(b)] are evident: First, SQF surfaces are *rougher* than ME surfaces and, second, all surfaces are quite *flat* for weak disorder. In previous work [14], we argued that for ME surfaces, there is a *transition* between a weak disorder phase (with perhaps logarithmic

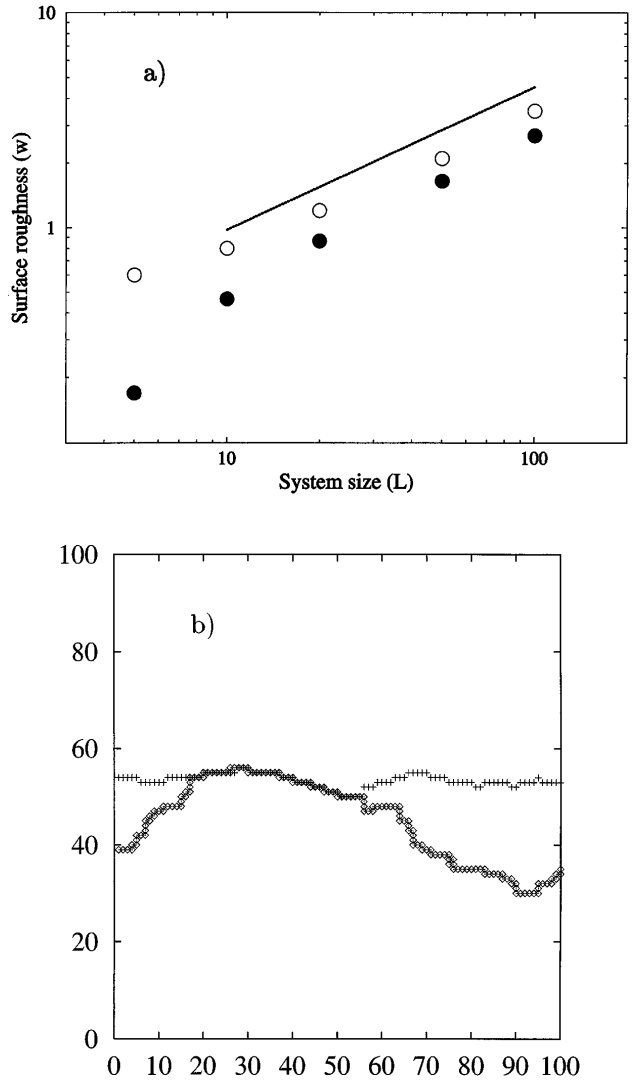

FIG. 2. The roughness w of scalar quasistatic fracture (SQF) surfaces and minimal energy (ME) surfaces in the {10} orientation square lattices for a *uniform distribution of disorder*. (a) Log-log plot of w versus L for $R = 1$: SQF (open circles); ME (filled circles). The dotted line has slope $\zeta = \frac{2}{3}$. For SQF, the number of configurations in the averages, N, varied from $N = 50$ for $L = 100$ to $N = 400$ for $L = 5$, while for the ME case, we used $N = 100$ for $L = 1000$ up to $N = 5000$ for $L = 10$. (b) (SQF) (diamonds) and ME (plus signs) surfaces in one configuration of a two-dimensional {10}, $L = 100$ random network with $R = 1$.

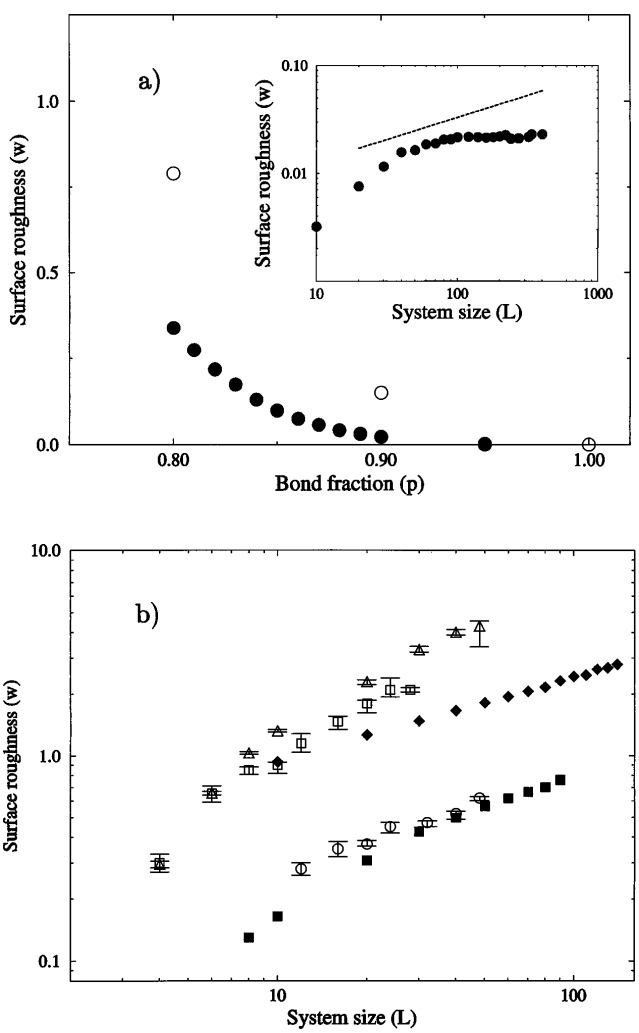

FIG. 3. The roughness w of SQF and ME surfaces in three dimensions. (a) w as a function of p for SQF ($L = 40$, $N = 30$—open circles) and ME ($L = 40$, $N = 5000$—solid circles) surfaces. The inset shows a finite-size-scaling plot of the roughness at $p = 0.90$, which is in the "weak disorder" regime. (b) Log-log plot of w in the "strong disorder" regime. Open symbols are for SQF surfaces and filled symbols are for ME surfaces. The data are for $R = 1$ (squares), $R = \frac{1}{2}$ (circles), $p = 0.7$ (triangles), and $p = 0.50$ (diamonds). As in Figs. 1 and 2, the ME surfaces are averaged over thousands of configurations, while the largest size SQF surfaces are averages over around 50 configurations.

roughness) for $p > p_* \sim 0.89$ and an algebraically rough phase $p < p_*$. We have done extensive tests of this hypothesis with a parallel version of our optimization algorithm [17] and typical results are presented in the inset of Fig. 3(a). In that figure, we present the roughness as a function of sample size (up to 400^3) at $p = 0.90 > p_*$. At $p = 0.90$, we expect a log-log plot of the roughness to level off indicating an absence of algebraic scaling of the roughness. This is clearly seen in the inset of Fig. 3(a) and confirms our hypothesis of a transition at $p_* < 0.90$.

A finite-size-scaling plot of the roughness of SQF and ME surfaces in *the strong disorder regime* is presented in Fig. 3(b). These data again show that, in three dimensions, SQF surfaces are *rougher* than ME surfaces. The ME data (solid symbols) reach the asymptotic exponent $\zeta_{3d} = 0.41 \pm 0.02$ [14,15,18] with the sample sizes that are available. Note, however, that at smaller sizes, the $R = 1$ ME data have a considerably larger slope in this log-log plot. The fracture data at $R = \frac{1}{2}$ show a very simple scaling with exponent 0.40 ± 0.05, which is consistent with the ME value.

We find that for intermediate disorder (e.g., $p = 0.80$) this behavior is typical of SQF surfaces. However, at stronger disorder the SQF data have strong size effects [see $p = 0.7$—open triangles, and $R = 1$—open squares in Fig. 3(b)]. Although the slope in these data is initially large, it continuously decreases. We have analyzed these data in several ways. It is evident that unless the data change their trend $\zeta < 0.50$. A more detailed analysis using finite-size scaling forms, and an analysis of a running exponent yields estimates close to 0.40. Though much larger sample sizes are necessary to reach the asymptotic regime for the $R = 1$ and $p = 0.70$ cases, the data in Fig. 3(b) are consistent with the simple conclusion that SQF and ME surfaces have the random-bond Ising exponents, and that there are stronger finite-size effects at stronger disorder.

Now, we discuss some reasons for the trends seen in the data of Figs. 1–3. Because of local current concentrations, one might expect cracks to become "flatter" as they become larger. However, a random void displaced a small vertical amount from a horizontal crack always makes the crack deviate, no matter how long the crack (provided the neck between the void and the crack is small enough or, on lattices, provided the void is big enough). Once the crack has wandered off the horizontal plane, it has a relatively weak memory for the horizontal plane (the stress or current field has a rather small gradient on the length scale of the roughness of the crack). This allows the crack to explore the energetically most favorable bonds to break, in a similar manner to a ME surface. In fact, there are mechanisms which can make a SQF surface *rougher* than a ME one. In particular, although the stress field has a weak *average* gradient in the process zone, its absolute value is high. This produces bond breaking in the process zone *ahead of the crack tip*. Since the crack propagates through this zone, the disorder it sees is larger than that of the pristine disordered system. This effect of *damage generation* is similar to what is observed in measurements of acoustic emission in slow fracture of 2D media [19]. Because of this effect, SQF surfaces can be rougher than ME surfaces with the same initial disorder. Note that although we might expect this mechanism to decrease with increasing sample size due to the size effects in damage, we are interested in the damage near the crack tip and the behavior of that quantity with sample size is unknown.

In summary, we find that SQF and ME surfaces at strong disorder have out-of-plane roughness exponents $\zeta_{2d} = \frac{2}{3}$ and $\zeta_{3d} = 0.41 \pm 0.02$. However, at smaller sample sizes, our SQF surfaces have an effective exponent which can be considerably larger than 0.41. We confirmed that, for ME surfaces in $3d$, there is a weakly rough to algebraically rough transition at $p \sim 0.89$. This implies that cracks can be quite flat along the low energy (cusp) directions of a crystal lattice.

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